Remarks on the Extended Characteristic Uncertainty Relations

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Three remarks concerning the form and the range of validity of the state-extended characteristic uncertainty relations (URs) are presented. A more general definition of the uncertainty matrix for pure and mixed states is suggested. Some new URs are provided.

In the recent papers [1, 2] the conventional uncertainty relation (UR) of Robertson [5] (which includes the Heisenberg and Schrödinger UR [4] as its particular cases) have been extended to all characteristic coefficients of the uncertainty matrix [2] and to the case of several states [1]. In this letter we present three remarks on these extended characteristic URs.

The first remark refers to the form of the extended URs [1]: we note that they can be written in terms of the principal minors of the matrices involved and write the entangled Schrödinger UR [1] in a stronger form. The second remark is concerned with the extension of the characteristic inequalities to the case of mixed states and non- Hermitian operators. The extension is based on the suitably constructed Gram matrix for n operators and mixed states. The characteristic inequalities for n non-Hermitian operators are in fact URs for their $2n$ Hermitian components. The last remark is about the domain problem of the operators involved in the URs. The proper generalization of the uncertainty matrix is suggested as the symmetric part of the corresponding Gram matrix. For pure states which are in the domain of all product of the operators involved this Gram matrix coincides with the Robertson matrix, and its symmetric part is equal to the conventional uncertainty matrix.

Let us first recall the Robertson UR for n observables (Hermitian operators) $X_1, \ldots, X_n$ and a state $|\psi\rangle$ and its particular case of $n = 2$. The Robertson UR is an inequality for the determinant of the uncertainty matrix σ (called also dispersion or covariance matrix),

$$\sigma_{jk} = \tfrac{1}{2}\langle\psi|(X_j X_k + X_k X_j)|\psi\rangle - \langle\psi|X_j|\psi\rangle\langle\psi|X_k|\psi\rangle \equiv \sigma_{jk}(\vec{X}; \psi), \tag{1}$$

and it reads

$$\det \sigma(\vec{X}; \psi) \geq \det \kappa(\vec{X}; \psi) \tag{2}$$

where $\kappa(\vec{X}; \psi)$ is the matrix of mean commutators, $\kappa_{kj}(\vec{X}; \psi) = (-i/2)\langle\psi|[X_k, X_j]|\psi\rangle$. For two observables X and Y one has $\det \sigma = (\Delta X)^2(\Delta Y)^2 - (\Delta XY)^2$, $\det \kappa = -\langle\psi|[X, Y]|\psi\rangle^2/4$, and the inequality (2) can be rewritten in the more familiar form of Schrödinger UR:

$$(\Delta X)^2(\Delta Y)^2 - (\Delta XY)^2 \geq \tfrac{1}{4}|\langle[X, Y]\rangle|, \tag{3}$$

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where ΔXY stands for the covariance of X and Y, $\Delta XY = \sigma_{XY}$, and $\Delta XX \equiv (\Delta X)^2$ is the variance of X. Robertson came to his UR by considering the non-negative definite Hermitian matrix R,

$$R_{jk} = \langle \psi \,|\, (X_j - \langle X_j \rangle)(X_k - \langle X_k \rangle) \,|\, \psi \rangle, \tag{4}$$

which was represented as $R = \sigma + i\kappa$ (the proof of (2) can be found also in [6]). In [2] it was noted that $\det \sigma$ and $\det \kappa$ are the highest order characteristic coefficients $C_n^{(n)}$ [7] of σ and κ and Robertson UR (2) was extended to all the other coefficients in the form $C_r^{(n)}\left(\sigma(\vec{X}; \psi)\right) \geq C_r^{(n)}\left(\kappa(\vec{X}; \psi)\right)$, $r = 1, \ldots, n$. In [1] a scheme for construction of URs for n observables and m states was presented. As an example of URs within this scheme the following extended characteristic URs for n observables X_j and m states $|\psi_\mu\rangle$ were established,

$$C_r^{(n)}\left(\textstyle\sum_\mu \sigma(\vec{X}; \psi_\mu)\right) \geq C_r^{(n)}\left(\textstyle\sum_\mu \kappa(\vec{X}; \psi_\mu)\right) \tag{5}$$

$$C_r^{(n)}\left(\textstyle\sum_\mu R(\vec{X}; \psi_\mu)\right) \geq \sum_\mu C_r^{(n)}\left(R(\vec{X}; \psi_\mu)\right). \tag{6}$$

Noting that the Robertson matrix in a state $|\psi\rangle$ can be represented in the form of a Gram matrix $\Gamma^{(R)}$ for n non-normalized states of the form $||\chi_j\rangle = (X_j - \langle X_j \rangle)|\psi\rangle$, $\langle X_j \rangle = \langle \psi | X_j | \psi \rangle$,

$$R_{jk} = \langle (X_j - \langle X_j \rangle)\psi \,|\, (X_k - \langle X_k \rangle)\psi \rangle \equiv \Gamma_{jk}^{(R)}, \tag{7}$$

it was suggested [1] that Gram matrices for other types of suitably chosen non-normalized states $||\Phi_\mu\rangle$ can also be used for construction of URs of the form (5) and (6) for several observables and states, including the case of one observable and several states. Let us recall that matrix elements Γ_{jk} of a Gram matrix Γ for n (generally non-normalized) pure states $||\Phi_j\rangle$ are defined as $\Gamma_{jk} = \langle \Phi_j | \Phi_k \rangle$, and Γ is Hermitian and non-negative definite.

The first remark on the extended URs (5) and (6) is that they follow from a slightly more simple URs in terms of the principal minors $\mathcal{M}(i_1, \ldots, i_r)$ [7] of matrices σ, κ and R:

$$\begin{aligned}
\mathcal{M}\left(i_1, \ldots, i_r; \textstyle\sum_\mu \sigma_\mu\right) &\geq \mathcal{M}\left(i_1, \ldots, i_r; \textstyle\sum_\mu \kappa_\mu\right), \\
\mathcal{M}\left(i_1, \ldots, i_r; \textstyle\sum_\mu R_\mu\right) &\geq \textstyle\sum_\mu \mathcal{M}(i_1, \ldots, i_r; R_\mu).
\end{aligned} \tag{8}$$

The validity of (8) can be easily inferred from the proofs of characteristic URs in [1, 2]. Let us remind that $\mathcal{M}(i_1, \ldots, i_n; \sigma) = \det \sigma$, and the n different $\mathcal{M}(i_1; \sigma)$ are equal to the diagonal elements of σ. URs (5) and (6) can be obtained as sums of (8) over all minors of order r, since the characteristic coefficient of order r is a sum of all minors $\mathcal{M}_r$, which here are non-negative. The advantage of the forms (5) and (6) is that the characteristic coefficients of a matrix are invariant under the similarity transformations of the matrix. For any Gram matrix and its symmetric and antisymmetric parts the inequalities (5), (6) and (8) are valid.

For two observables X and Y and two states $|\psi_1\rangle$ and $|\psi_2\rangle$ the highest order inequalities (8) (the second order) coincide with the inequalities (5) and (6) and produce the state-entangled UR

(18) of ref. [1], which, after some consideration, can be written in the stronger form

$$\tfrac{1}{2}\left[(\Delta X(\psi_1))^2(\Delta Y(\psi_2))^2 + (\Delta X(\psi_2))^2(\Delta Y(\psi_1))^2\right] - |\Delta XY(\psi_1)\Delta XY(\psi_2)|$$
$$\geq \tfrac{1}{4}\left|\langle\psi_1|[X,Y]|\psi_1\rangle\langle\psi_2|[X,Y]|\psi_2\rangle\right|. \qquad (9)$$

For equal states, $|\psi_1\rangle = |\psi_2\rangle = |\psi\rangle$, the inequality (9) recovers the old Schrödinger UR (3).

The second remark is, that the extended URs related to any Gram matrix admit generalizations to mixed states and to non-Hermitian operators as well. For n non-Hermitian operators Z_j and a mixed state ρ we define a matrix $\Gamma^{(R)}(\vec{Z};\rho)$ as a Gram matrix for the transformed states $\tilde{\rho}_j = (Z_j - \langle Z_j\rangle)\sqrt{\rho}$ by means of the matrix elements of the form

$$\Gamma^{(R)}_{jk}(\vec{Z};\rho) = \mathrm{Tr}\left[(Z_k - \langle Z_k\rangle)\,\rho\,(Z_j^\dagger - \langle Z_j\rangle^*)\right]. \qquad (10)$$

These matrix elements can be represented as Hilbert-Schmidt scalar products $(\cdot,\cdot)_{\mathrm{HS}}$ for the transformed states $\tilde{\rho}_j$,

$$\Gamma^{(R)}_{jk}(\vec{Z};\rho) == \mathrm{Tr}\left[\tilde{\rho}_k\tilde{\rho}_j^\dagger\right] = (\tilde{\rho}_k,\tilde{\rho}_j)_{\mathrm{HS}}, \qquad (11)$$

For pure state $\rho = |\psi\rangle\langle\psi|$, $(\tilde{\rho}_k,\tilde{\rho}_j)_{\mathrm{HS}} = \langle(Z_j - \langle Z_j\rangle)\psi\,|\,(Z_k - \langle Z_k\rangle)\psi\rangle$. When a cyclic permutation $\mathrm{Tr}(Z_k\rho Z_j^\dagger) = \mathrm{Tr}(Z)j^\dagger Z_k\rho)$ is possible, then

$$\Gamma^{(R)}_{jk}(\vec{Z};\rho) = \mathrm{Tr}\left[(Z_j^\dagger - \langle Z_j\rangle^*)(Z_k - \langle Z_k\rangle)\,\rho\right] \equiv \langle(Z_j^\dagger - \langle Z_j\rangle^*)(Z_k - \langle Z_k\rangle)\rangle, \qquad (12)$$

and $\Gamma^{(R)}(\vec{X};\rho)$ coincides with the Robertson matrix: $R(\vec{X};\rho) = \sigma(\vec{X};\rho) + i\kappa(\vec{X};\rho)$.

Thus $\Gamma^{(R)}(\vec{Z};\rho)$ with elements given by eq. (10), is a generalization of the Robertson matrix to the case of non- Hermitian operators and mixed states.

For several mixed states ρ_μ the Gram matrices $\Gamma^{(R)}_{jk}(\vec{Z};\rho_\mu)$, and their symmetric and antisymmetric parts $S(\vec{Z};\rho_\mu)$ and $K(\vec{Z};\rho_\mu)$, whose matrix elements take the form

$$S_{jk}(\vec{Z};\rho_\mu) = \mathrm{Re}\left[\mathrm{Tr}(Z_k\rho_\mu Z_j^\dagger)\right] - \mathrm{Re}(\langle Z_j\rangle^*\langle Z_k\rangle),$$
$$K_{jk}(\vec{Z};\rho_\mu) = \mathrm{Im}\left[\mathrm{Tr}(Z_k\rho_\mu Z_j^\dagger)\right] - \mathrm{Im}(\langle Z_j\rangle^*\langle Z_k\rangle), \qquad (13)$$

satisfy the extended characteristic inequalities (5) and (6). We have to note that the characteristic inequalities for $S(\vec{Z};\rho_\mu)$, $K(\vec{Z};\rho_\mu)$ and $\Gamma^{(R)}(\vec{Z};\rho)$ can be regarded as new URs for the $2n$ Hermitian components X_j and Y_j of Z_j, $Z_j = X_j + iY_j$. The simplest illustration of this fact is the case of two boson annihilation operators $a_j = (q_j + ip_j)/\sqrt{2}$ and one state. For $n = 2$ the second order characteristic coefficient $C_2^{(2)}$ is the determinant of the corresponding matrix. After some consideration we obtain $\det K(a_1, a_2;\rho) = (\Delta q_1 p_2 - \Delta q_2 p_1)^2/4$, and

$$\det S(a_1, a_2;\rho) = [(\Delta q_1)^2 + (\Delta p_1)^2][(\Delta q_2)^2 + (\Delta p_2)^2]/4 - (\Delta q_1 q_2 + \Delta p_1 p_2)^2/4. \qquad (14)$$

The characteristic inequality $\det S(a_1, a_2;\rho) \geq \det K(a_1, a_2;\rho)$ takes the form of a new UR for q_1, q_2, p_1 and p_2,

$$[(\Delta q_1)^2 + (\Delta p_1)^2][(\Delta q_2)^2 + (\Delta p_2)^2] \geq (\Delta q_1 q_2 + \Delta p_1 p_2)^2 + (\Delta q_1 p_2 - \Delta q_2 p_1)^2. \qquad (15)$$

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The above consideration suggests that the symmetric part $S(\vec{X}, \rho)$ of $\Gamma^{(R)}(\vec{X}; \rho)$ (defined in eq. (10) with $\vec{Z} \to \vec{X}$) could be taken as a *generalized definition of the uncertainty matrix* for n observables X_j in mixed state ρ.

The third remark concerns the equivalence of the expressions (10) and (12) for the Gram matrix. They are equivalent if the cyclic permutation of the operators $Z_k \rho Z_j^\dagger$ in the trace $\mathrm{Tr}(Z_k \rho Z_j^\dagger)$ is possible. For $\rho = |\psi\rangle\langle\psi|$ this is rewritten as $\langle Z_j \psi | Z_k \psi \rangle = \langle \psi | Z_j^\dagger Z_k \psi \rangle$ and it means that the state $|\psi\rangle \in \mathcal{D}(Z_j Z_k)$, where $\mathcal{D}(Z_j Z_k)$ is the domain of the operator product $Z_j Z_k$. However it is well known that this not always the case. Example is the squared moment operator $p^2 = -d^2/dx^2$ and any state represented by a square integrable function $\psi(x)$ which at some points has (first but) no second derivative. In this sense the expression (10) is more general than (12). Then the symmetric part $S(\vec{X}; \psi)$ of $\Gamma^{(R)}(\vec{X}; \psi)$ is to be considered as more general definition of the uncertainty matrix in pure states, and $S(\vec{X}; \rho)$, eq. (13) with $\vec{Z} = \vec{X}$, – in mixed states.

After this work was completed I learned about the very recent E-print [8], where (in view of the domain problem) the expression $\mathrm{Re}\langle X\psi \,|\, Y\psi \rangle - \langle X \rangle\langle Y \rangle$ is proposed as a more general definition of the covariance of the Hermitian operators X and Y in a pure state $|\psi\rangle$.

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